Communications

Comments on a Recent Infinitesimal-Deformation Approach to Martensite Crystallography*

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Recently, Navruz[1] gave a reformulated infinitesimal-deformation approach to martensite crystallography, and he applied it to the fcc-to-bct transformation in Fe-7Al-2C.[2,3] That study contained three claims: (1) a better prediction of the shape-deformation magnitude m_1; (2) "excellent" agreement with predictions of the Wechsler–Lieberman–Read/Bowles–Mackenzie (WLR/BM) invariant-plane-strain theories,[4,5] and (3) (implied) a simpler alternative to the WLR/BM theories.

Here, we dispute all of these claims.

The first, and simplest claim is dismissed easily. Navruz claimed that his predicted shape-deformation magnitude $m_1 = 0.1274$ agrees better with observation (0.1220) than the WLR/BM value, 0.1379. However, Watanabe and Wayman[3] estimated a large error (20.8 pct) in their measured m_1; thus, $m_1 = 0.1220 \pm 0.0253$. Their measurement bounds include both the WLR/BM and Navruz predictions.

Second, as for "excellent" agreement between Navruz's theory and WLR/BM, we focus on the habit plane **p**, which is more sensitive than the orientation relationships discussed by Navruz. Although Navruz calculated **p**, he failed to point out the 7.3 deg discrepancy between his prediction and the average observed **p**. This is a large discrepancy. Habit planes are usually measured within 1 deg, and prediction-observation agreement is often within a few degrees. Because Navruz did not report the shape-change direction **d**, or sufficient information to compute it, we cannot compare his **d** prediction with the WLR/BM prediction, which would provide another sensitive test. Figure 1 shows the observed, Navruz, and WLR/BM **p** results plotted in the standard unit triangle. (The WLR/BM **p** coordinates given by Navruz are incorrect, and about 7 deg from the correct WLR/BM prediction.)

Third, Figure 1 also shows a curious feature of Navruz's **p** prediction: it is confined to the $(0\ k\ l)$ line, as shown also by the expressions for **p** in his Table II. One lesson from the WLR/BM theories and the related measurements is that habit planes are irrational with general indices $(h\ k\ l)$. The value $h = 0$ imposes a severe constraint. Thus, the Navruz formulation must fail increasingly as habit planes move away from the $(0\ k\ l)$ curve. Other formulations of the infinitesimal-deformation approach also encounter the $(0\ k\ l)$ dilemma, for example, Khachaturyan[6] and Mura *et al.*[7]

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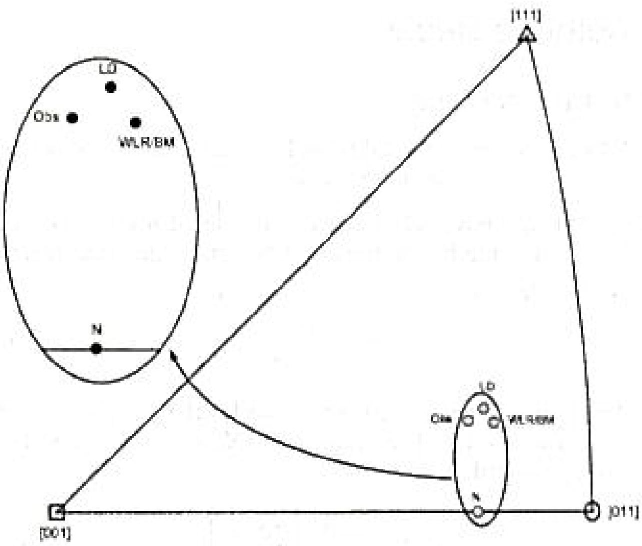

Fig. 1—Stereographic plot of habit-plane normals **p**. Navruz point is confined to the $(0\ k\ l)$ line 7.3 deg from observation. The WLR/BM point is 1.7 deg from observation. The Ledbetter–Dunn point is 1.7 deg from observation, taking a twinning fraction of 0.40. For the WLR/BM case, the twinning fraction is 0.38. If the martensite-plate aspect ratio is increased slightly from zero, the Ledbetter–Dunn theory gives *exact* agreement with observation.

Using an infinitesimal-deformation approach, Ledbetter and Dunn[8] found that $\mathbf{p} = (0\ k\ l)$ if the lattice-invariant deformation is neglected. Later,[9] they showed that a correct treatment of the lattice-invariant deformation moves the predicted **p** from $(0\ k\ l)$ through the unit triangle up to the $(h\ h\ l)$ line, that line corresponding to equal twin volumes. Thus, we conclude that the Navruz formulation is confined to predict $(0\ k\ l)$ habit planes near (011) and provides no useful alternative to the WLR/BM invariant-plane-strain approaches nor to the Ledbetter–Dunn infinitesimal-deformation approach, which includes WLR/BM as a special case, the zero-elastic-strain-energy case.[10] Figure 1 also shows the prediction of the Ledbetter–Dunn theory.

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Author's Reply

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I do not accept the validity of Ledbetter and Dunn's comments for the following reasons:

(1) When a physical quantity is measured n times (x_1, x_2, ... x_n), the best estimate of the true value (the mean) is given by

$$X_n = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad [1]$$

Any particular measurement, x_i, will differ from the mean value by an error. The accuracy of X_n as an estimate of x_i is the standard error,[1] $\sigma(X_n)$:

$$\sigma(X_n) = \frac{1}{\sqrt{n}}\left[\sum_{i=1}^{n} \delta_i^2\right]^{1/2} \qquad [2]$$

where δ_i, the deviation of each measurement is

$$\delta_i = x_i - X_n \qquad [3]$$

Thus, the results of an experiment are given in the form

$$X = X_n \pm \sigma(X_n) \qquad [4]$$

Using Watanabe and Wayman's 11 measurements for magnitude of the shape deformation listed in Table II,[2] the mean value from Eq. [1] and the standard error from Eq. [2] are obtained:

$$m_1 = 0.1220 \pm 0.0072 \qquad [5]$$

Thus, the error in their measurements is 5.9 pct, unlike the 20.8 pct claimed by Ledbetter and Dunn. As can be clearly seen, Ledbetter and Dunn's expression, $m_1 = 0.1220 \pm 0.0253$, is incorrect. As a result, since experimental bounds include only Navruz predictions,[3] Navruz predictions and comments on m_1 are valid.

(2) The habit planes given by Navruz are the undistorted planes. As known, in WLR theory,[4] the undistorted habit plane is given in the form $\frac{1}{\sqrt{1+K^2}}(0\ 1\ K)$. In order to make meaningful comparisons with theoretical predictions and observations, the habit plane must be unrotated as well as undistorted. The undistorted plane (**p**) and the invariant plane (**p**′) are related by the matrix Γ; therefore,

$$\mathbf{p}' = \Gamma\mathbf{p} \qquad [6]$$

where

$$\Gamma = \begin{pmatrix} 0.980191 & 0.198060 & 0 \\ 0.198056 & 0.980190 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad [7]$$

for the fcc → bct martensitic transformation with the (110) $[\bar{1}10]$ slip system in the Fe-7 pct Al-2 pct C alloy.

Therefore, their comments on the habit plane are not valid.

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